Optimizing Lab Operations: Integrating Laboratory Instruments and Calculations with LIMS

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INTRODUCTION

Laboratories are facing significant competitive pressures to increase productivity with fewer resources, and the primary avenue to achieve this goal is through automation. Laboratory automation includes the integration of Laboratory Information Management Systems (LIMS) with equipment such as instrumentation and associated calculations. With this approach, laboratories can experience the following benefits:

1. Eliminate the need for manual data entry, producing time savings
2. Enhance data quality by removing the potential for transcription errors
3. Reduce resource drain associated with having highly trained analysts performing data entry
4. Assist with regulatory compliance with enforcement of instrument maintenance and calibration information
5. Enable business scalability in terms of throughput and growth
6. Facilitate future changes in workflow with minimized efforts
7. Drive cost savings through improved speed and efficiency across the laboratory

Instrument Types and LIMS Interface Requirements

Instruments fall into three general classes, identified by the communication mechanism:

- Simple
- Direct (Uni-Directional)
- Bi-Directional (Import/Export)

Simple:

Simple instruments such as balances and pH meters are widely used, but do not provide a direct way to correlate the required reference to its associated record within the LIMS database (e.g. the unique sample identifier and parameter name). Rather, they provide an electronic output via an RS232 or USB port, which means the LIMS must provide a way to acquire the data and convert it into a compatible format. This process is generally straightforward in a traditional local area network (LAN) environment, where the instrument and LIMS are hosted on the same network but becomes more complicated in a web environment where these pieces must be able to communicate with a remote server across the Internet or a corporate Intranet.

Fortunately, this task can be simplified by employing an application such as the Confience Bridge, which includes web services that can communicate with desktop applications.

To facilitate this process, the web service passes data between the LIMS database and the client-side application. The client-side application then connects the instrument to the PC, provides a client-interface, acquires and parses the data, and passes the data from the instrument back to the web service.

Direct (Uni-Directional):

Direct instruments, also known as uni-directional, operate on a one-way communication system from the instrument to the LIMS, and provide two key features that simplify interfacing to the LIMS:

1. They allow you to associate the unique sample identifier to each measurement.
2. They provide files in a format that can be processed by software applications.

The format of the files that are produced will vary greatly; some use modern, common formats such as XML or CSV that are simple to process, while others use proprietary text layouts that must be parsed to extract the necessary data. Files that are generated from the instrument are exported to a web server where they may be processed via a LIMS web service that extracts the appropriate data and parses it to the LIMS database. This includes both raw data and final results.

Bi-Directional (Import/Export):

Like direct/uni-directional instruments, import/export instruments, more commonly referred to as bi-directional instruments (Figure 1), allow the input of sample identification and produce files that contain the instrument-produced data in a consistent format. Additionally, these instruments provide the added capability of sharing information directly from the LIMS in the form of a Worklist. For example, Worklists can be generated within the LIMS and passed to the instrument directly, allowing the analyst to load the instrument and run the analysis. Upon completion of the analysis, the data is sent back to the LIMS automatically, to complete the bi-directional communication cycle.

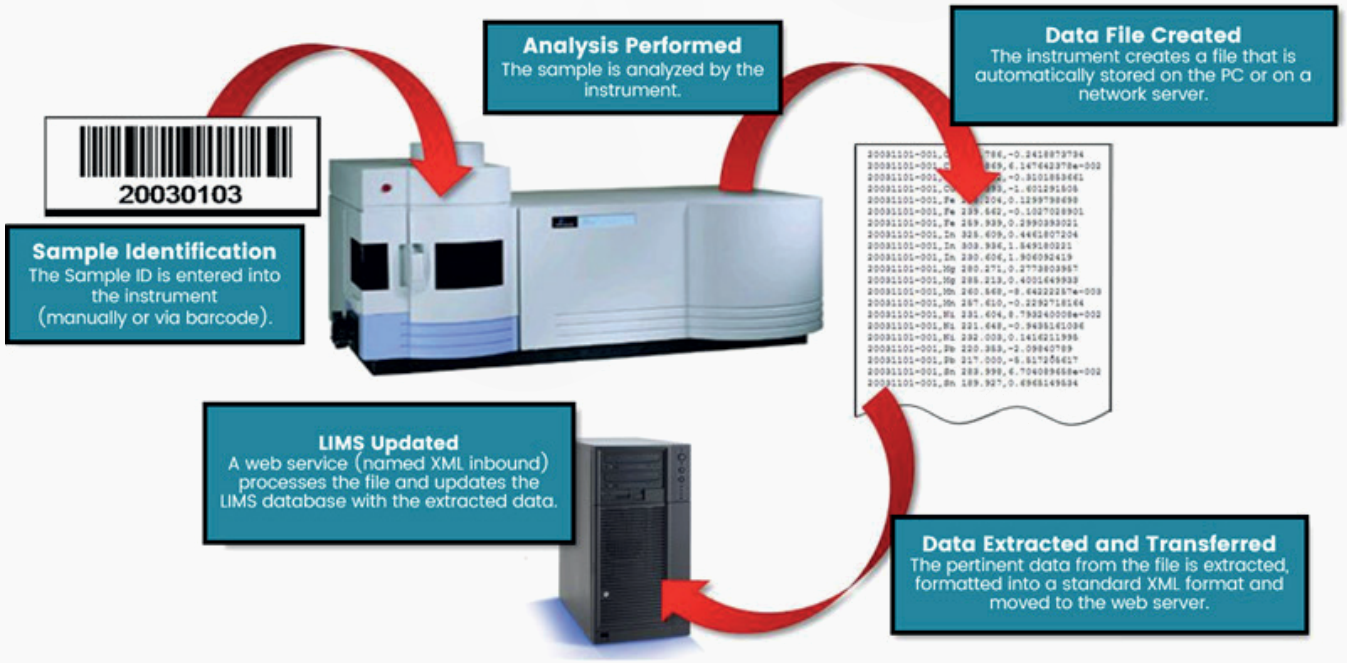

Figure 1 - Instrument Interfacing – Bi - Directional Instrument Processing Cycle

Because instrument manufacturers do not provide common communication or data formats, a tool, such as the Confience LIMS Bridge (Figure 2) is needed. The LIMS Bridge supports the creation and update of samples, analytical results and virtually any other type of information used by the LIMS that originates from external sources such as analytical instruments, process control systems and Excel spreadsheets, among others. The LIMS Bridge also delivers information from the LIMS to the instrument/system, ensuring a closed communications loop that increases productivity and minimizes errors, supporting faster and more accurate results.

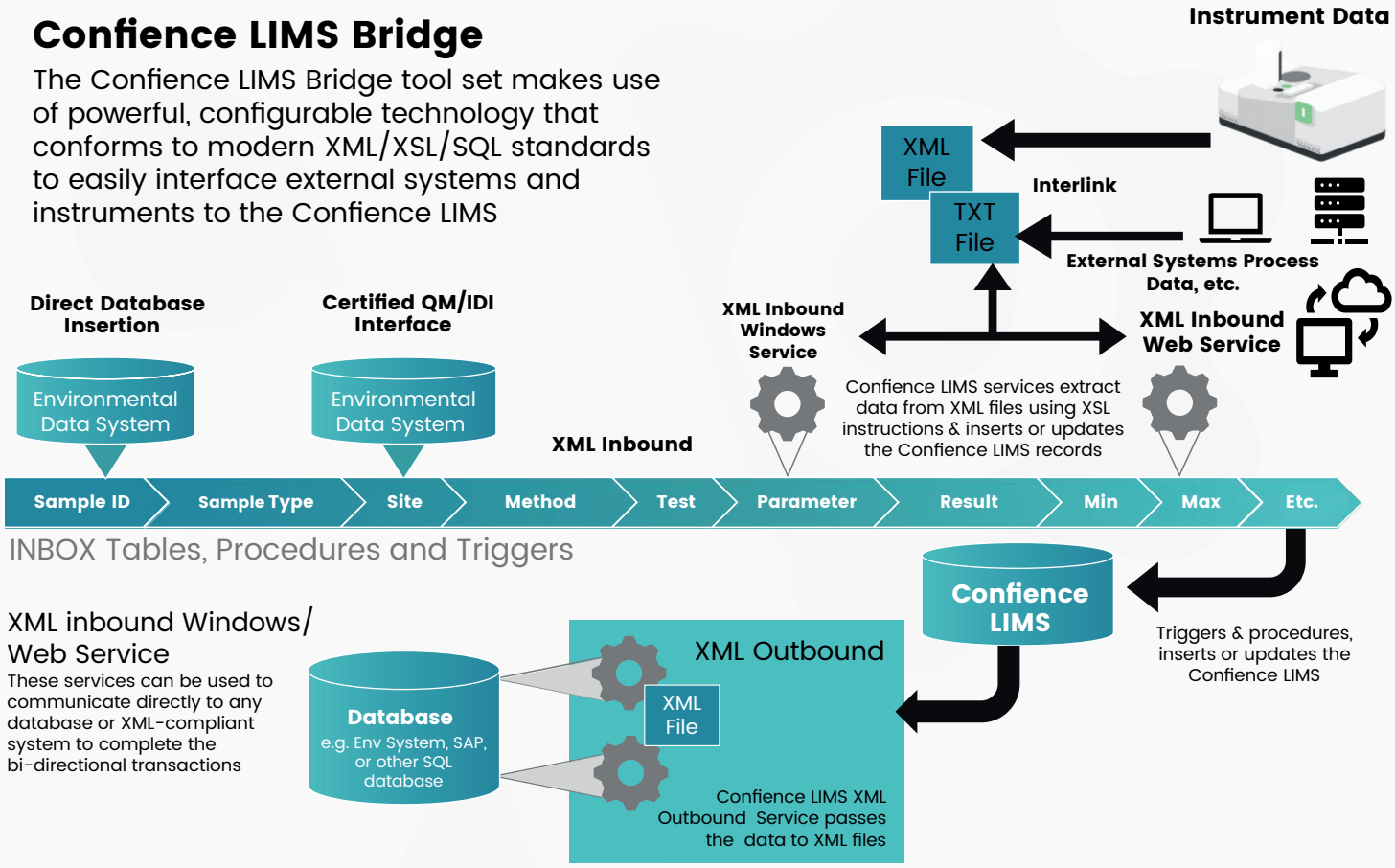

Figure 2 – Confience LIMS Bridge Tool

Imported Result Validation

Integration allows for real-time monitoring of instrument performance and results, supporting immediate identification and resolution of issues. As instrument data is populated into the LIMS, results are checked against all predefined limits. Color-coded cells alert users when values have exceeded the predefined warning limits.

With integration, the most common types of transcription errors including transposition of information, rounding values incorrectly, or applying limits improperly, are minimized.

Sample #	Product Code	Test Method	Parameter	Result	Units	Spec Min	Spec Max	Typical/Targe
Q622	200.8 Metals - Direct Analysis (blar	200.8 Metals - Direct Analysis	Zinc	<1.80	µg/L		0.00500	0.000
Q623	200.8 Metals - Direct Analysis (low	200.8 Metals - Direct Analysis	Aluminum	<1.00	µg/L	0.900	1.10	1.00
Q623	200.8 Metals - Direct Analysis (low	200.8 Metals - Direct Analysis	Antimony	1.01	µg/L	0.900	1.10	1.00
Q623	200.8 Metals - Direct Analysis (low	200.8 Metals - Direct Analysis	Arsenic	<1.40	µg/L	0.900	1.10	1.00
Q623	200.8 Metals - Direct Analysis (low	200.8 Metals - Direct Analysis	Barium	0.990	µg/L	0.900	1.10	1.00
Q623	200.8 Metals - Direct Analysis (low	200.8 Metals - Direct Analysis	Beryllium	0.993	µg/L	0.900	1.10	1.00
Q623	200.8 Metals - Direct Analysis (low	200.8 Metals - Direct Analysis	Cadmium	0.959	µg/L	0.900	1.10	1.00
Q623	200.8 Metals - Direct Analysis (low	200.8 Metals - Direct Analysis	Chromium	1.03	µg/L	0.900	1.10	1.00
Q623	200.8 Metals - Direct Analysis (low	200.8 Metals - Direct Analysis	Cobalt	1.02	µg/L	0.900	1.10	1.00
Q623	200.8 Metals - Direct Analysis (low	200.8 Metals - Direct Analysis	Copper	1.03	µg/L	0.900	1.10	1.00

Figure 3 = Results Validation

Instrument Calibration & Control

Integrated LIMS functionality allows users to define and closely monitor each of the instruments used for analyzing samples and provides an on-line means for tracking all instrument maintenance, scheduling of maintenance events and on-line recall of past maintenance events.

In addition, this functionality enables users to record results from all calibration and QC samples run on each instrument and maintain this data online for monitoring both usage and performance. This also supports regulatory compliance requirements.

Instant SQC charts for each instrument may be generated to provide a clear, graphical illustration of instrument performance, identify trends and to allow users to take a proactive role in preventing instrument-related issues.

Automated Calculations

Confience eLIMS includes a Derived Results Calculation Engine (Figure 4) with exceptional flexibility that allows calculation routines that can use numeric values from anywhere within the LIMS tables, enabling techniques such as “cross sample” calculation, i.e. the ability to incorporate results from one sample in the calculation of results for another.

An example of this might be the application of correction coefficients tracking the performance of an analysis against calibration standards to correct results “on the fly” at any time in a series of measurements.

Examples of a few of the calculations that can be incorporated into a LIMS include the following:

- Cation/Anion Balance
- % Moisture - Calculate this from % solids and enter it into the appropriate records for all parameters in the results entry form
- % Recovery
- RPD (Relative Percent Difference)
- Volume corrected RDL (Report Detection Limit)
- % Solids
- Total Suspended Solids

- Dissolved Solids
- Total Nitrogen (TKN + NO2 + NO3)
- Dry Weight basis results
- Alkalinity (calculated from Calcium and Magnesium results)
- Cetane Rating for fuels
- API Gravity from Specific Gravity
- Langlier Index

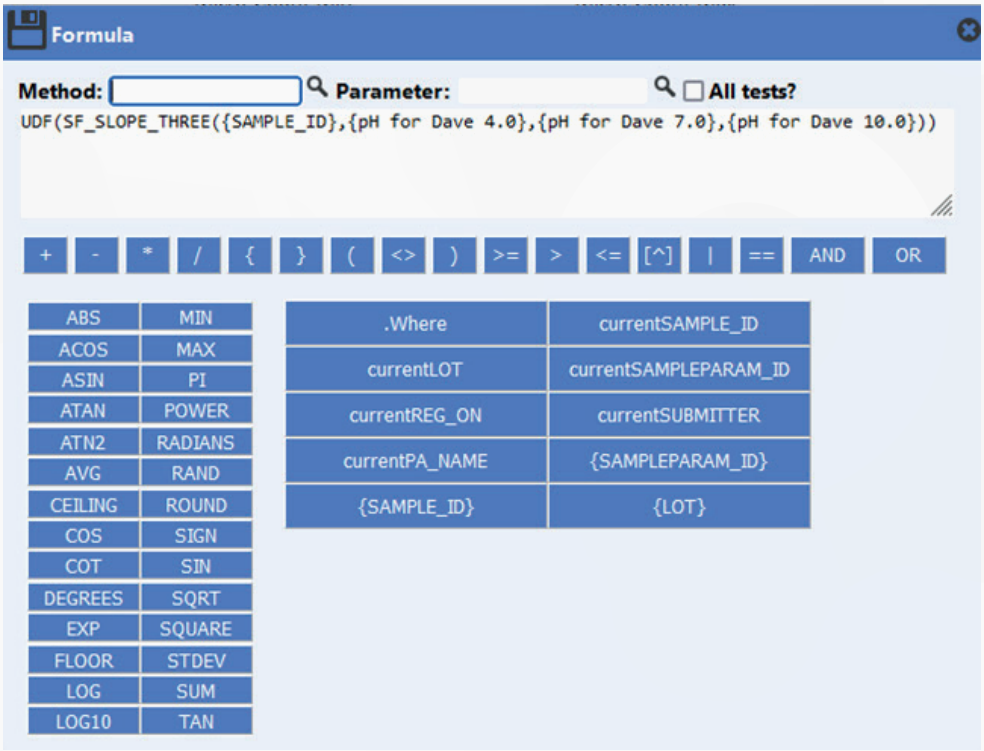

Figure 4 - Results Calculation Engine

LIMS users are encouraged to incorporate as many calculations as possible, as automating calculations facilitates error reduction and efficiency.

Costs Associated with Instrument Integration

Many vendors charge fees for integrating instruments with the LIMS.

Instrument interfacing software, such as Confience LIMS Bridge, enables end users to configure their own interfaces to instrument output files, spreadsheets or 3rd party data acquisition tools. This cost-effective option often provides the payback required to justify the purchase of your LIMS software.

In certain highly regulated environments, additional costs may be associated with system validation per audit guidelines, validation documentation, or additional configuration and training.

Automating data collection and integration reduces the need for manual labor, decreasing personnel costs and allowing staff to focus on more complex and value-added tasks rather than routine data handling.

The long-term benefits of increased efficiency, improved data accuracy, and enhanced productivity often justify the expense incurred with LIMS implementation and instrument integration.

Resource Savings

The automatic data transfer from laboratory instruments to the LIMS eliminates the need for manual data entry and significantly reduces the time required to record results. Integration of automatic calculations and instruments facilitates smoother workflows by reducing downtime between different stages of experiments and analyses, ensuring a more continuous and efficient operation.

Another area of savings is in the sample set up exchange between the LIMS and the instrument. The LIMS can export a worklist to the instrument so that the instrument knows the order in which the samples are to be analyzed. Once analysis is completed, the instrument can then return the results, with their associated samples, to the LIMS in the same order.

Worklists can be sent to the instrument controller for:

- Pre-configuring instrument runs
- Pre-generating instrument run worklists
- Calculations
- Result checking
- Direct reporting to the LIMS
- Archiving
- Organized data files
- Automated user defined automatic import to the LIMS

Examination of data generated by Confience customers has demonstrated that there is a linear trend when the number of samples are analyzed over time. During the configuration phase, the laboratory analysts and the QC managers must decide how best to implement the integration, as it is not always desirable to have instrument runs set up automatically.

In Figure 5, we have plotted the number of tests (analyses) per day (average number of samples per day, multiplied by the average number of parameters for each test per sample) against the number of hours that are saved per day. There is a clear trend that emerges - the higher the volume of samples, the higher the number of hours saved. There is a major divergence when it comes to samples with associated calculations, and our analysis has shown 2-4 times the savings, depending on the calculation's complexity.

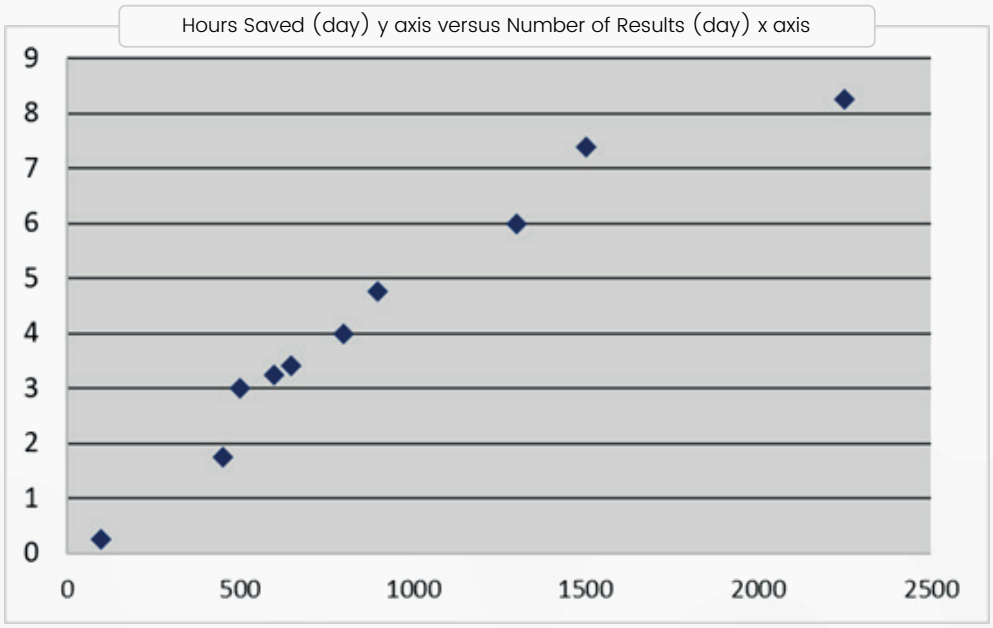

Figure 5 - Number of Tests Per Day vs. Number of Hours Saved Per Day

Faster data capture and processing leads to quicker analysis and reporting, reducing the overall turnaround time.

SUMMARY

Integrating laboratory instruments and calculations with LIMS offers substantial benefits, enhancing accuracy, efficiency, compliance, and decision-making. This strategic investment not only modernizes operations but also strengthens a laboratory's competitive edge. For labs seeking improved efficiency and competitiveness, such integration is a smart choice.